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Title: The Development of a Lagrangian Cloud Microphysics Package in HiGrad
for the Simulation of PyroCumulonimbus (PyroCb) Clouds

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The Development of a Lagrangian Cloud Microphysics Package in HiGrad for the Simulation of Pyrocumulonimbus (PyroCb) Clouds

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Introduction to HiGrad: High Gradient Model

- Developed at LANL for over 20 years
- Includes several modules and subroutines to model:
 - Clouds
 - Hurricanes
 - Wildfire-atmosphere interactions (when coupled with FIRETEC)
 - Explosives behavior
- Solves compressible Euler equations in 3-space in generalized coordinates

Conservation of mass, momentum, energy:

$$\partial_t \mathbf{u}(\mathbf{x}, t) + \partial_x \mathbf{F}(\mathbf{u}(\mathbf{x}, t)) = \mathbf{0}, \quad \mathbf{x} \in \mathcal{I}, \quad t > 0,$$

$$\mathbf{u}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}), \quad \mathbf{x} \in \mathcal{I}, \quad t = 0,$$

$$\mathbf{u} = \begin{pmatrix} \rho \\ m \\ E \end{pmatrix} \text{ and } \mathbf{F}(\mathbf{u}) = \begin{pmatrix} m \\ \frac{m^2}{\rho} + p \\ \frac{m}{\rho}(E + p) \end{pmatrix}$$

and

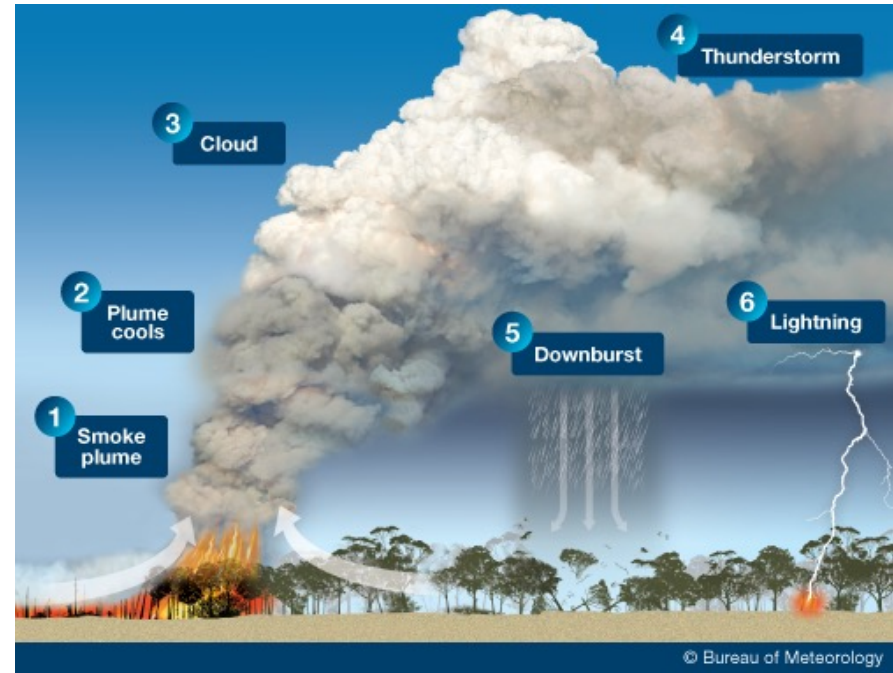
$$\mathbf{u}_0(\mathbf{x}) = \begin{pmatrix} \rho_0(\mathbf{x}) \\ m_0(\mathbf{x}) \\ E_0(\mathbf{x}) \end{pmatrix}$$

Equation of State:

$$p = (\gamma - 1) \left(E - \frac{m^2}{2\rho} \right)$$

Pyrocumulonimbus (PyroCb) Clouds

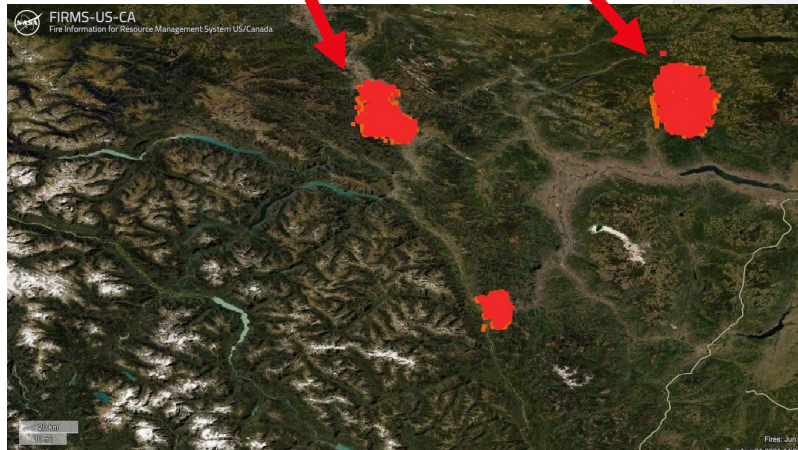
- Form by condensation of intensely heated, rising air becoming saturated due to adiabatic cooling
 - Lifting provided by buoyancy due to heat + moisture from fire + latent heat release from phase change
- Extent of pyroCb development depends on atmospheric stratification + ambient moisture + fire fluxes of heat and moisture
- Can produce lightning and precipitation
- Intense updrafts can carry significant quantities of smoke and aerosols into stratosphere



https://media.bom.gov.au/social/upload/images/pyrocumulus_Blog.png

Why do we want to model PyroCbs?

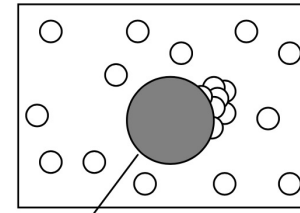
- Motivation: Sparks Lake Fire, BC



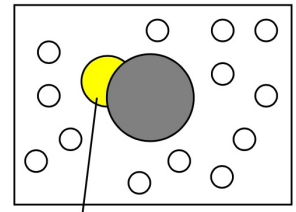
Important to be able to capture microphysical processes in our numerical simulations to more accurately depict and study these phenomenon

Cloud Microphysics Overview

Heterogeneous Nucleation: water condenses onto micron and sub micron aerosol particles in the atmosphere that serve as “condensation nuclei”



Non-soluble foreign particle



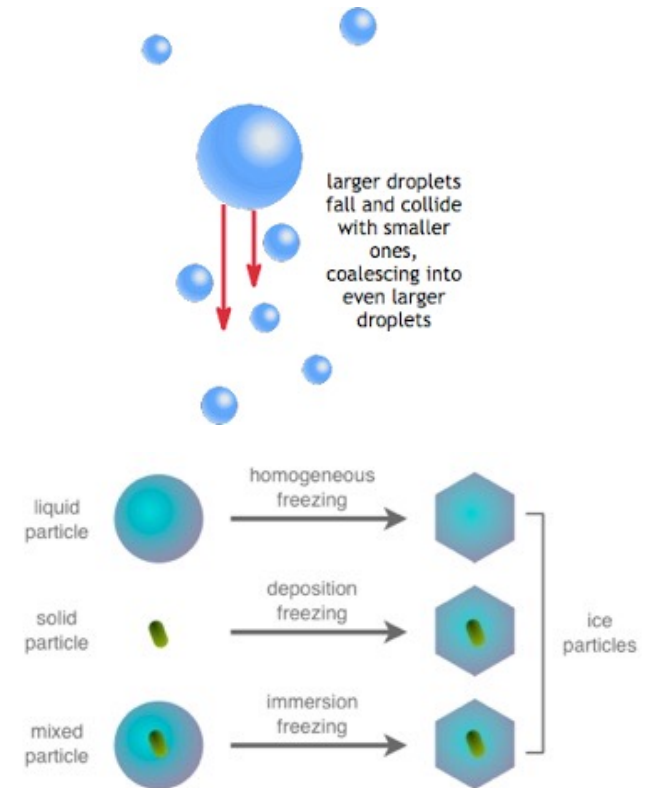
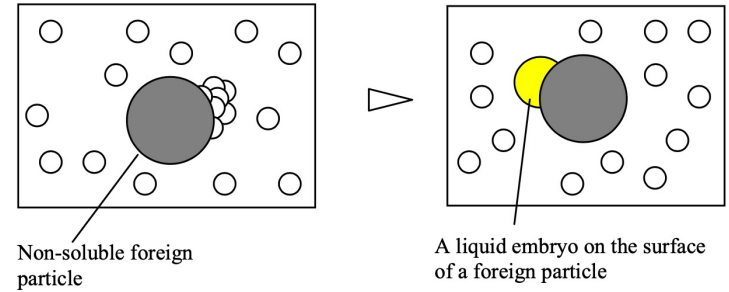
A liquid embryo on the surface of a foreign particle

Cloud Microphysics Overview

Heterogeneous Nucleation: water condenses onto micron and sub micron aerosol particles in the atmosphere that serve as “condensation nuclei”

Collision and Coalescence

Ice Crystal Formation and Growth



Cloud Microphysics Overview

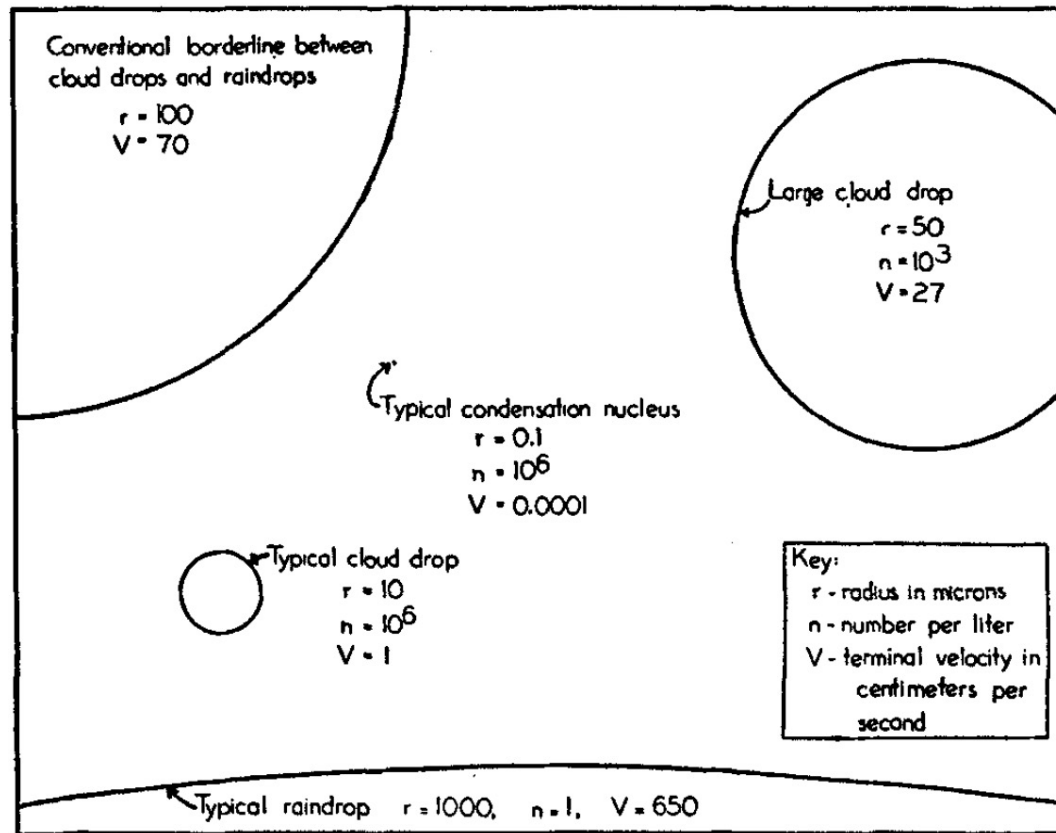


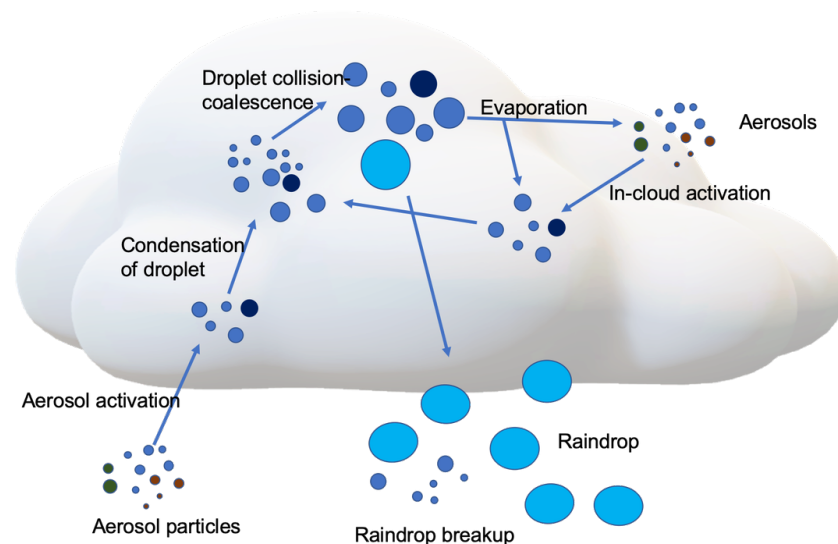
FIG. 2. Comparative sizes, concentrations, and terminal fall velocities of some particles involved in condensation and precipitation processes. Note particularly the great difference in radius of a typical cloud drop and of a typical raindrop.

Statement of Research Problem and Goals

- Modeling development of clouds and precipitation processes involves sub-centimeter scale referred to as **cloud microscale**
- Most atmospheric models apply Eulerian approach for clouds with thermodynamics variables
- Most common and efficient method used today is Lagrangian Cloud Model (LCM)
 - Eulerian flow-field + Lagrangian framework to capture microphysics

Statement of Research Problem and Goals

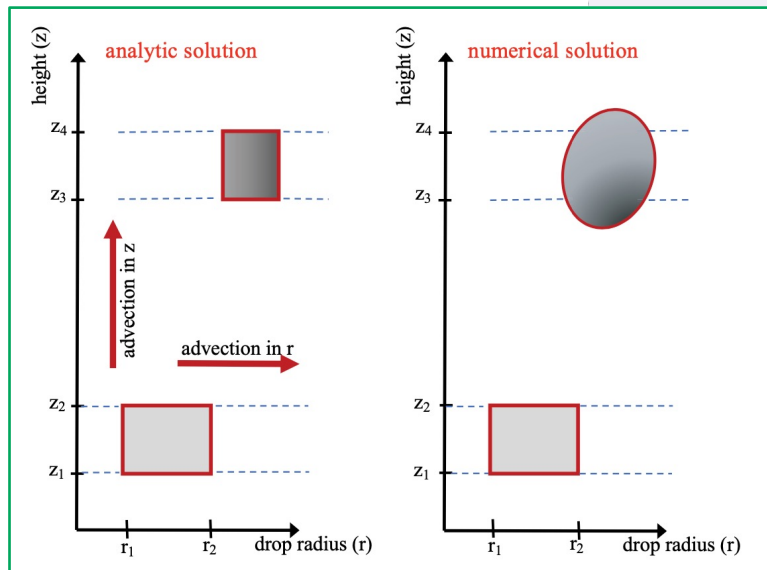
- Implement Lagrangian Cloud Model within HiGrad that can simulate the following microphysical cloud processes within a pyroCb event:
 - Aerosol (soot) production and tracking
 - Condensation of water onto aerosols as they rise
 - Evaporation of water droplets
 - Collision/coalescence of water droplets
 - Ice nucleation
 - Raindrop breakup



Why Lagrangian Cloud Microphysics

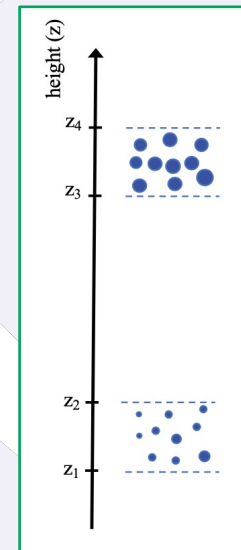
• Classic Eulerian Approach

- Explicitly model evolution of particle size/mass distributions
- Numerical diffusion leads to unphysical broadening of particle size distributions
- Increasing complexity of microphysical interactions has not shown convergence of model results



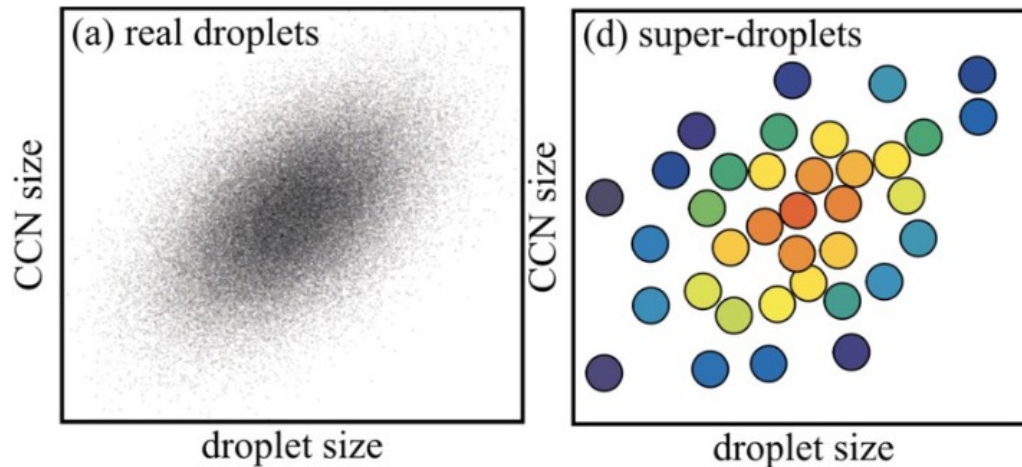
• Lagrangian Approach

- Combine group of cloud droplets with same properties into a superdroplet; track specific superdroplet's evolution in time
- No numerical diffusion because transport in physical space and growth of droplets calculated individually using ODEs
- Simulates relationship between aerosol and cloud droplet number concentration with accuracy compared to observed data



Lagrangian Cloud Microphysics

- Superdroplet Method (SDM): combines group of cloud droplets with same properties into a superdroplet (SD)
- Ensemble of SDs traced in physical space using model-predicted flow field and grown or shrink as they move with the flow
- SDs experience all cloud microphysical processes in the model



The Lagrangian Cloud Model: Activation + Condensation

Background aerosol: condensation nuclei not particularly of interest

Activation criteria: initialized as $r = 1$ micron superdroplets and immediately start growing

Condensation:

$$\frac{dr}{dt} = \frac{GSF}{r}$$

$$G = \frac{1}{F_k + F_d} \quad F_k = \left(\frac{l_v}{R_v T} - 1 \right) \frac{l_v}{qT} \quad \text{Heat conduction term} \quad F_d = \frac{R_v T}{De_S(T)} \quad \text{Vapor diffusion term}$$

$$D = (0.015T - 1.93) \quad \text{Diffusivity of water vapor}$$

$$e_S(T) = 6.112e^{\frac{17.67T}{T+243.5}} \quad \text{Saturation vapor pressure}$$

$$S = \frac{q_v}{q_{vs}} - 1 \quad \text{Supersaturation}$$

$$F \quad \text{Ventilation Factor } (\sim 1)$$

R_v	Moist gas constant
q	Thermal conductivity of moist air
T	Temperature
l_v	Latent heat of vaporization
q_v	Water vapor mixing ratio
q_{vs}	Saturation water vapor mixing ratio

The Lagrangian Cloud Model: Activation + Condensation

Source aerosol: organic carbon and black carbon (soot)

Activation criteria: initialized as $r = 100$ nanometer superdroplets and start growing based on κ

Condensation:

$$r \frac{dr}{dt} = \frac{D_{eff}}{\rho_w} (q_v - q_{vs} a_w(r, r_d, \kappa) \exp\left(\frac{A}{r}\right))$$

Effective Diffusion term:

$$\frac{1}{D_{eff}} = (D\rho_d)^{-1} + K^{-1} q_{vs} \frac{l_v}{T} \left(\frac{l_v}{R_v T} - 1 \right)$$

Kohler term:

$$A = \frac{2\sigma_w}{R_v T \rho_w}$$

Water activity:

$$a_w(r, r_d, \kappa) = \frac{r^3 - r_d^3}{r^3 - r_d^3(1 - \kappa)}$$

ρ_w	Density of liquid water
ρ_d	Density of dry air
D	Diffusivity of water vapor
K	Heat conduction term
T	Temperature
l_v	Latent heat of vaporization
q_v	Water vapor mixing ratio
r	radius
r_d	Dry radius
κ	Hygroscopicity parameter
q_{vs}	Saturation water vapor mixing ratio
σ_w	Surface tension of water
R_v	Moist gas constant

The Lagrangian Cloud Model

Background aerosol + Source aerosol

Evaporation criteria: (performed every timestep, for every superdroplet)

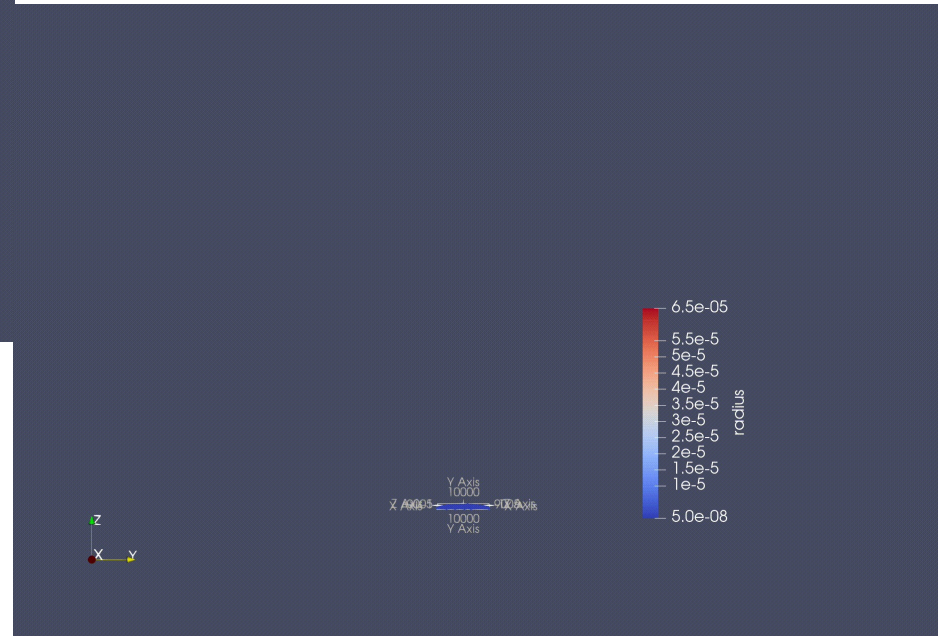
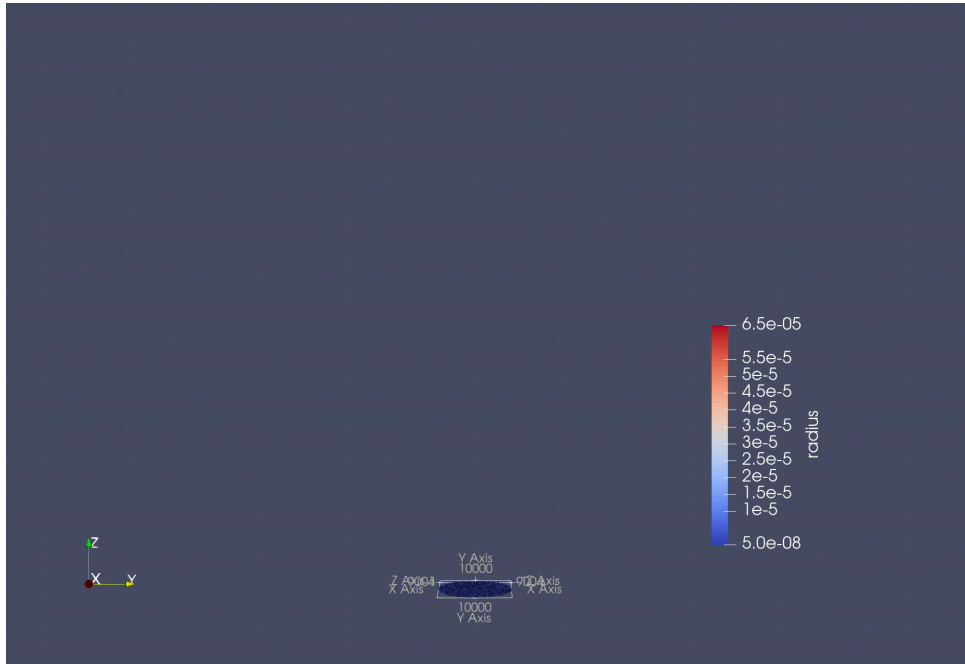
$$\text{If } \frac{r_w - r_d}{r_d} < 0.01, \text{ then evaporate}$$

Multiplicity (m) values: how many real particles represented by superdroplet

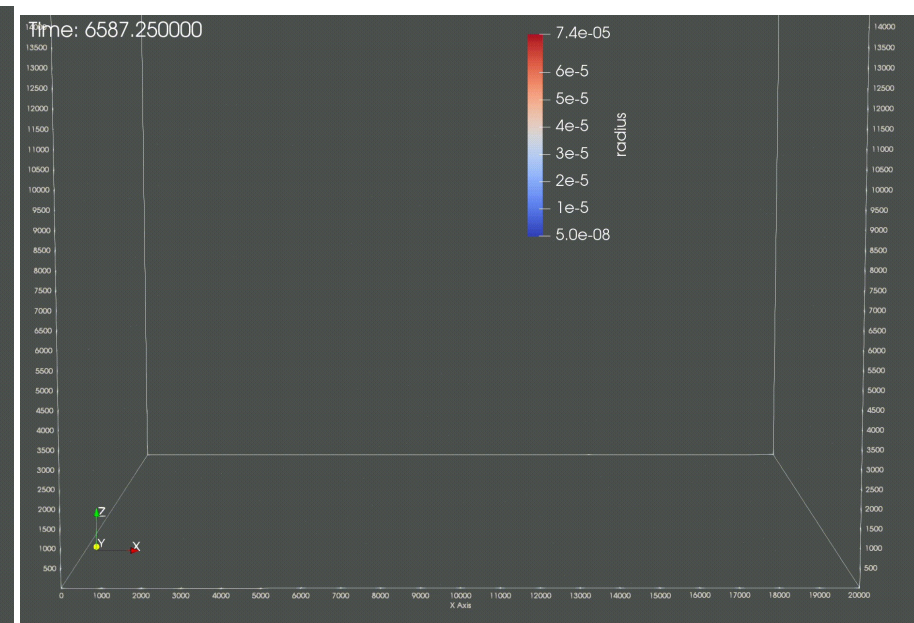
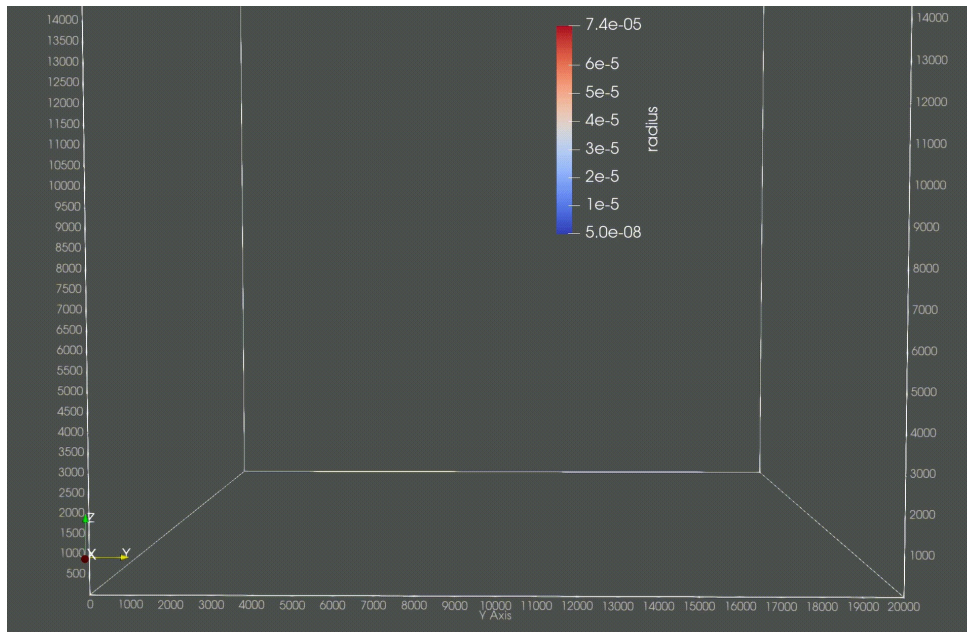
$$9 \times 10^{12} < m < 2 \times 10^{14}$$

The Lagrangian Cloud Model Preliminary Results: Activation, Condensation, Evaporation

Cross section:

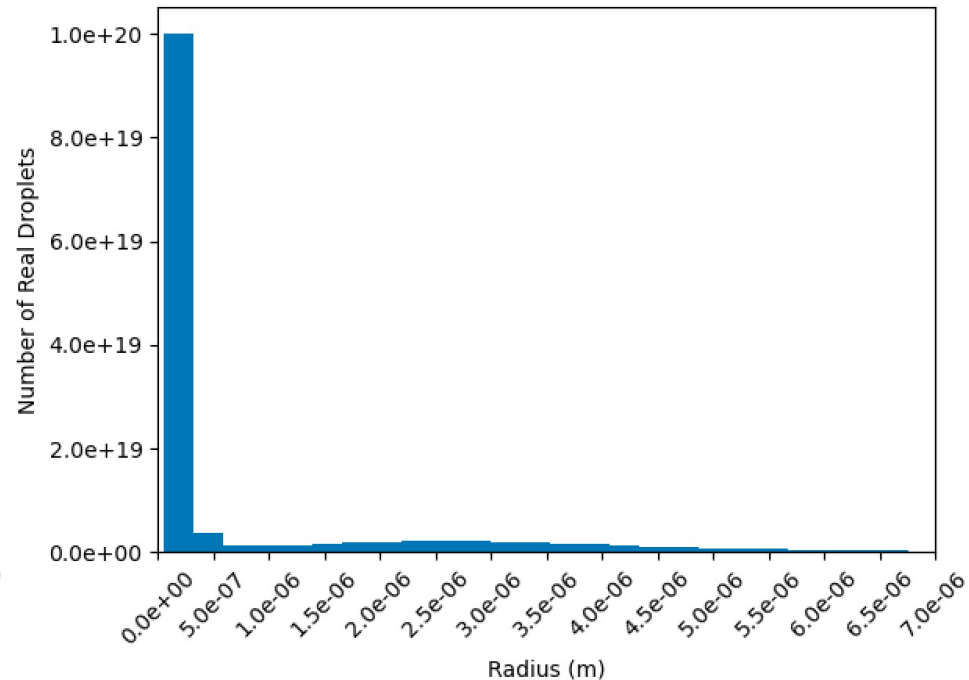
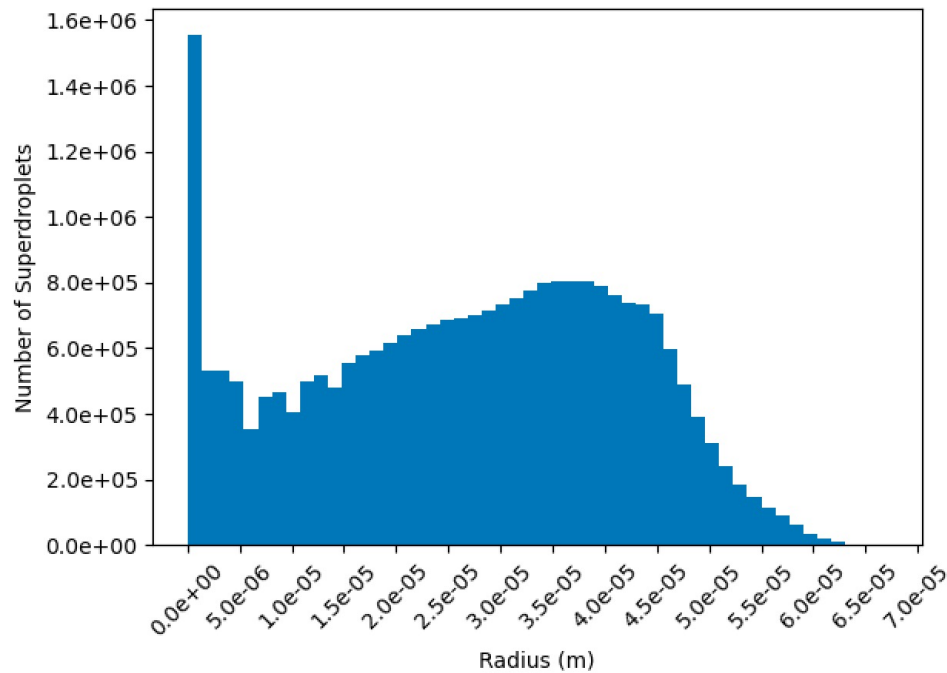


The Lagrangian Cloud Model Preliminary Results: Particle Tracking



The Lagrangian Cloud Model Preliminary Results:

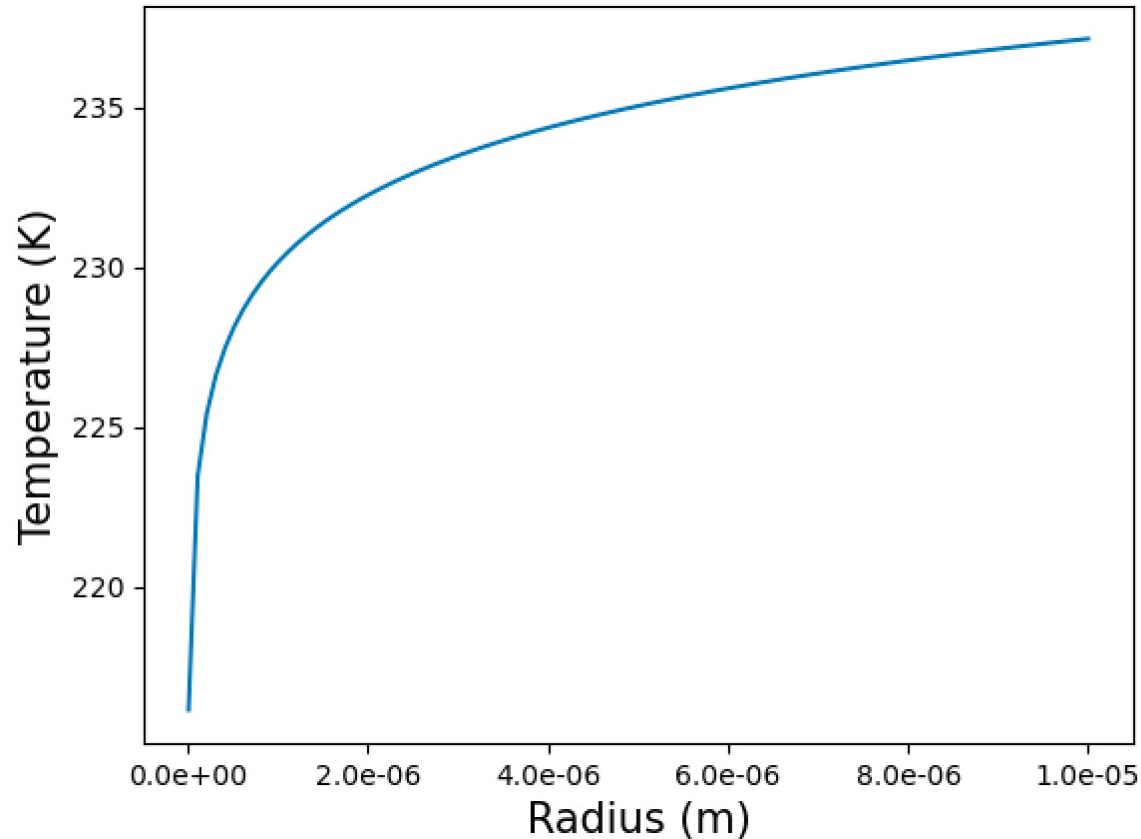
Particle Size Distribution



Measurements from Literature	Cloud Droplet Diameter
2002 Amazon Deforestation Fires, Martins and Dias(2009)	< 30 microns
2018 Western US Fire Season, Twohy et al.(2021)	5 - 7 microns
2002 Amazon Deforestation Fires, Andreae et al.(2004)	< 40 microns
WRF Simulation Idealized Supercells, Kalina et al.(2014)	< 18 microns
WRF Simulation Deep Convective Systems in China, Xie et al.(2013)	5.5 - 9 microns
WRF Supercell Storm Simulation, Lim et al.(2011)	5 - 25 microns
Measurements of Supercell Thunderstorm in Montana, Musil et al.(1986)	< 30 microns

Next Step: Ice Microphysics

- Implement freezing of liquid cloud droplets according to



Future Work

- Ice microphysics
 - Important for initiation of precipitation
- Collision/Coalescence of droplets
 - Important for the formation of rain droplets
- Raindrop breakup
 - Important for modeling precipitation
- Soot liquid water content (LWC) for atmospheric chemistry applications
- Simulation of Sparks Lake Fire from BC 2021 Fire Season with all microphysical processes

Thanks! Questions?

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Kohler term:

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Water activity:

$$a_w(r, r_d, \kappa) = \frac{r^3 - r_d^3}{r^3 - r_d^3(1 - \kappa)}$$

Diffusivity of water vapor:

$$D = D_0 \frac{1 + \frac{\lambda_D}{r}}{1 + 1.71 \cdot \frac{\lambda_D}{r} + 1.33 \cdot \left(\frac{\lambda_D}{r}\right)^2}$$

Heat conduction term:

$$K = K_0 \frac{1 + \frac{\lambda_K}{r}}{1 + 1.71 \cdot \frac{\lambda_K}{r} + 1.33 \cdot \left(\frac{\lambda_K}{r}\right)^2}$$

Latent heat of vaporization:

$$l_v(T) = l_{v0} + (c_{pv} - c_1)(T - T_0)$$

$$\lambda_D = 2D_0(2R_v T_w)^{-\frac{1}{2}}$$

$$\lambda_K = \frac{4}{5} K_0 \frac{T}{p} (2R_d T)^{-\frac{1}{2}}$$

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T	Temperature
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